

## Synchrotron X-Ray Studies of Soft Matter and Biomolecular Materials: Small Angle Scattering (SAXS) Using the NSLS X21 Beamline

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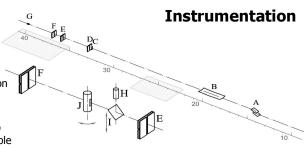
§ Wiggler source + cryogenicallycooled monochromator (A) with interchangeable Si(111) and multilayer elements

§ Toroidal focusing mirror (B)

 ${\mathbb S}$  Vacuum-compatible high precision slits (D-F), beam monitor (H) and shutter (J)

 $\,$  5-20KeV, ~10^{10}ph/s (Si) or up to 11KeV, ~10^{12}ph/s(ML) at the sample





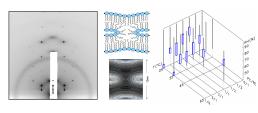


## **Self-assembled lipid structures**

Small angle x-ray scattering (SAXS) and diffraction at grazing incidence and in transmission geometry are used to study various periodic structures lipids form in the presence of water. Studying these structures not only helps to understand self-assembly of soft materials, but also provides insight to the physics behind the biological processes that involve lipid membranes.

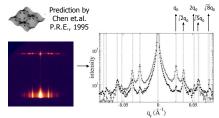
### Spontaneous curvature and fusion

Electron density distribution calculated from the diffraction pattern of DPhPC (branched chains) R phase showed stalks, an intermediate structure during bilayer fusion, trapped in a rhombohedral lattice. Interestingly, the appearance of this structure in DOPC/PE (C18:1 chains) mixtures can be controlled by tuning the spontaneous curvature (mixing ratio of PC:PE) of the lipid layer.



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#### Square modulated phase

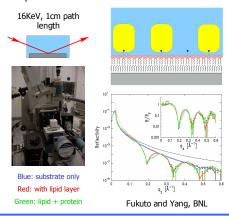


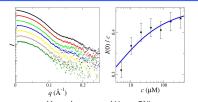
Yang and Fukuto, NSLS

DTPC (C13:0) form a layered structure with in-plane square modulations. The diffraction data from this structure confirms the theoretical consideration that the coupling between bilayer shape and local chain tilt leads to layer shape modulation, but also suggests that other factors, e.g. interbilayer interaction may also play a role.

# **Substrate-supported** bilayer

The formation of a lipid bilayer on the silicon substrate under water and the subsequent adsorption of proteins can be monitored by x-ray reflectivity (XR). Working at relatively high x-ray energy reduces the absorption by the sample.



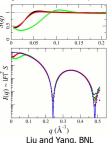


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#### Particles in solution

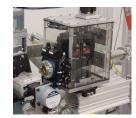
SAXS data from solutions that contain identical particles contain information on not only the structure of particle, but also the interaction between them. In the example above above, a

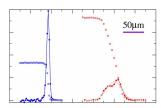
protein is measured at a series of concentrations to determine its dimer dissociation constant. On the right, the pHdependent interaction nano-shells between manifests as the 🗟 variation the in measured structural factor S(q).



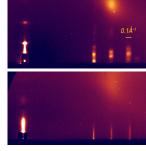
## Molecular packing in organic thin films

Grazing incidence diffraction (GID) at wide angles reveals molecular packing in organic thin films. CCD-based measurements are much faster than those using Soller slits and a linear detector. The sample therefore suffers less radiation damage. However, the q-resolution usually deteriorates at wide scattering angles because of the parallex effect induced by the finite beam footprint on the sample. At X21, this problem is alleviated by a secondary vertical focusing mirror that reduces the vertical beam size to  $\sim 7\mu m$  (FWHM).





A micro-focusing mirror is used to reduce the vertical beam size, greatly improves angular resolution in GID, as clearly shown by example data from pentacene films (top: unfocused beam, bottom: focused beam).



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